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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). This project was motivated by the recognition that we have entered a golden age for exploiting complex electronic materials based on discoveries and techniques totally beyond traditional solid state. The new materials are characterized by strong competitions between coupled electronic, structural and magnetic degrees-of-freedom, and large sensitivities to dimensionality and geometry. Tuning these competitions and sensitivities by chemistry, pressure, magnetic fields, doping, temperature, etc., controls macroscopic functionalities that will enable next-generation civilian and defense technologies.

To move towards a comprehensive capability in this critical underpinning science, this project established regular joint experimental-theoretical meetings, and prompted extensive LANL discussion of approaches to structure-function relations in modern materials, under the rubric of "complex adaptive matter". We developed modeling techniques for polarons, and charge-ordering in transition metal perovskite oxides, and new methods for calculating transport in nonequilibrium and nonadiabatic polaron systems, retaining full quantum coherence. We analyzed impurity-induced quasi-particle gap states in novel superconductors. We calculated metal-insulator/magnetic transitions and transport in colossal magneto-resistance perovskites. We analyzed new crossover effects of interchain coupling in spin-Peierls systems. We extended data analysis techniques based on information entropy, and analyzed signatures of local structure available from new high-intensity neutron and light sources.

Background and Research Objectives

We have entered a golden age for exploiting complex electronic materials based on discoveries totally beyond traditional solid state—heavy fermions, conducting polymers, high-temperature superconductors, fullerenes, quantum Hall effect and quantum well systems, etc. The new materials are characterized by strong competitions between coupled electronic, structural and magnetic degrees-of-freedom, and sensitivities to dimensionality and geometry. Tuning these microscopic competitions by chemistry, pressure, magnetic fields, temperature, light, etc., controls intrinsic complexity at mesoscopic scales, which in turn controls macroscopic functionalities (optical, magnetic, electronic properties). The unusual ground and excited states are just beginning to be utilized in niche technologies but there are vast markets for next generation materials if the new science is fully implemented, controlled and utilized for optoelectronics, sensors, recording, refrigeration, etc., as well as

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for fundamental relationships to coupled structural and electronic complexity in materials such as Pu and its alloys. Los Alamos has been, over the last 15 years, an international center of excellence for interdisciplinary research in correlated electron physics, as witnessed by the many honors received and our ability to attract major consultants (such as nobel laureate Robert Schrieffer) and superb young staff, postdocs and students.

This underpinning skill-base has been the fundamental driving force for our rapid entry at Los Alamos into, and leadership in, competitive fields such as high-temperature superconductivity, polymer light-emitting diodes, colossal magnetoresistance, thermoelectric refrigeration, relaxor ferroelectrics, high-magnetic field research, etc. These fields are now launched on specific technology tracks with limited support for sustained basic research. There is a compelling need and opportunity to do much more for the future. Stretching this *de facto* competency will provide seed corn for many future spin-offs such as those above.

This project was tightly coupled to the companion experimental project "Synthesis and Characterization of Correlated Electron Materials". In an integrated team approach our principal goals were to: (1) isolate novel phenomena that must be controlled for new technology challenges; (2) integrate synthesis-characterization-modeling teams to study those phenomena in specific classes of materials; and (3) develop improved scientific control of synthesis-microstructure-property.

Importance to LANL's Science and Technology Base and National R&D Needs

Los Alamos not only must retain but stretch its world-class competency to systematically control tunable classes of correlated electron materials for targeted technology issues. With dwindling resources this is clearly becoming the approach to R&D on many-body electronic materials nationally. By history, reputation and infrastructure, Los Alamos is the ideal environment to lead this national agenda, involving industry, universities and national laboratories. Of the major national laboratories, Los Alamos is unique in both its breadth and depth in correlated electron materials. No other institution has the combined abilities to develop new materials, characterize them and carry out theoretical modeling at all levels. Correlated electron physics is a scientifically vital area of research that continues to excite the imagination and challenge our physical intuition, and at the same time opens new avenues of electronics applications for industrial and defense technologies where the anticipated United States annual product is in the multi-billion dollar range. This thrust has helped to maintain and stretch Los Alamos' competency in advanced and nuclear materials, in particular, those in which electronic correlations play a dominant role, and provide the scientific basis for ideas that we and the nation will "mine" for the

technologies of the next century. We have laid the path for working synergistically with industry, agencies, universities and other national labs to develop a focus for (a) identifying key classes of novel electronic materials possessing characteristics defined by industrial and weapons roadmaps and (b) controlling the fundamental science issues for optimization of the identified characteristics. We have shown the value of developing new theoretical and modeling tools and strategies as appropriate, and working closely with synthesis and characterization programs to "close-the-loop" — this is key to the holy grail of predictive control for synthesis-microstructure-property relations.

This project, combined with its experimental companion, utilized unique Laboratory facilities and leveraged existing programs. In addition we have used programs in the Center for Materials Science (CMS), the Superconductivity Technology Center (STC), the Center for Nonlinear Science (CNLS), and with the University of California (UC) to provide a national focus through workshops and visitors involving industry, universities and other national laboratories.

Scientific Approach and Accomplishments

The fundamental R&D need is to successfully "close-the-loop" of synthesis-characterization-modeling around critical scientific issues. This requires a dedicated interdisciplinary and multi-technique team of skilled researchers who are also closely aware of broad technology issues and challenges—our staff are all simultaneously involved in shorter-term technology teams and thus have the mechanisms to both appreciate such issues and transfer new insights in a timely manner. We focused on critical scientific issues; classes of materials and phenomena; optimizing use of unique Laboratory facilities; involvement of researchers with proven track-records and team strengths, and exploring industry/university/lab interactions.

Correlated electron behavior is especially prominent at the magnetic-nonmagnetic boundary in d- and f-electron materials, typically accompanied by a metal-insulator transition. There is a progression from localized (heavy rare earths and actinides) to itinerant (4d, 5d) electronic behavior. The progression is accompanied by varying degrees of coupling among spin, charge and lattice degrees-of-freedom. These couplings lead to a vast variety of broken-symmetry ground states (charge and spin density, superconducting, ferroelectric, charge ordered, etc.). For applications, we must control these ground states, transitions between them, and transitions to metallic phases— the basis of, e.g., heavy-fermion superconductivity and magnetism, cuprate superconductivity, catalytically active materials, magnetoresistive transition-metal manganites, and the coupling of electronic and

structural "texture" complexity of Pu alloys (whose science must be understood for forming and aging, just as in other martensitic-like materials).

We focused on three critical science issues recognized to be at the cutting edge of international research in correlated electron physics:

(a) What are the roles of electron-electron and electron-lattice interactions, disorder, restricted geometries and dimensionalities, chemical doping, magnetic field, pressure and temperature in controlling metal-insulator transitions in correlated electron materials.

(b) What conditions induce unusual non-Fermi liquid metallic behavior and what are the experimental signatures and consequences?

(c) How can multiple (mesoscopic) scales of local structure be probed with NMR, XAFS, pair-distribution function analysis of x-ray/neutron diffraction data? It is now critical to go beyond global structure analysis (Rietveld), but totally new nonlinear nonadiabatic protocols must be developed and connections with optical and vibrational signatures understood.

We studied these three issues in representative materials (d- and f-electron heavy-fermion intermetallics, perovskite-like 3d-electron oxides, and martensitic/elastic surrogates for Pu alloys) whose understanding will impact a much larger class of correlated electron materials (e.g., organic charge-transfer salts, multilayer magnetic materials, shape-memory alloys). Through these materials, we provided some of the underpinnning science for key technologies, including the future of programs in, e.g., high-temperature superconductivity, colossal magnetoresistance, ferroelectrics, high-magnetic field phenomena, active oxide thin films, science-based stockpile stewardship (e.g., aging of Pu), and thermoelectric refrigeration.

In theory and modeling, we took advantage of the Advanced Computing Laboratory (ACL) and other Los Alamos high-performance computing strengths with which we were already well-integrated. No single technique or simulation is capable of handling the complexity of strongly correlated electronic materials. We, therefore, continued our successful approach of seeking new many-body techniques which merge traditional approaches from solid-state physics and quantum chemistry; a combination of state-of-the-art analytical and numerical schemes. The strength of the Los Alamos many-body modeling capability lies in its unusually broad coverage of all these techniques—it is their cross-fertilization that has led to many new modeling breakthroughs in the last decade. We purposefully aimed to "close-the-loop" for understanding and control by introducing minimal many-body models for classes of materials with coupled degrees-of-freedom, determining model parameter values from approximate calculations, solving the models by

the above multi-technique approach, predicting ground and excited state properties (electronic, magnetic, structural, optical), and testing the predictions against precise experiments on controlled materials. The experimental input then acts to refine parameter values or extend minimal models and the process can be iterated.

To move toward our objectives we have undertaken a number of important organizational and science advocacy steps: (i) Establishing a regular discussion team between relevant staff in the Materials Science and Technology (MST) and Theoretical (T) Divisions, which has focused attention on our "closing-the-loop" perspective and highlighted new directions and current issues for the experimental-theoretical team; (ii) Promoting the importance of coupled "charge-lattice-spin" effects in complex electronic materials, especially transition metal oxides—as witnessed by our invited talks at the March APS Meetings (1996, 1997, 1998), Gordon Conferences, and international Conferences [including "Spin-charge-lattice coupled phenomena in perovskite oxides" (Tsukuba, Japan 1996), "Correlated electrons" (Institute for Theoretical Physics, UCSB 1996), "Lattice dynamics and phase transitions" (Ettore Majorana Center, Erice, Sicily 1997), "Stripes 98" (Rome, Italy 1998), Aspen Center for Physics Program (Aspen, Colorado 1998)—see Publications for a complete list]; (iii) Emphasizing the importance of coupled structural and electronic complexity in Pu alloys, etc., as part of the developing Laboratory debate to study the important underpinning science for stockpile stewardship.

We have been very successful in working synergistically with the project on "Correlated Electron Materials" including joint visitors throughout the year; interaction with Fellows R. Schrieffer, D. Pines, J. Wilkins, E. Abrahams, Z. Fisk, and D. Scalapino; and coordination with its Summer Workshops. We hosted a very successful International Workshop on "Spin-Charge-Lattice Coupling" (August 1997) at Los Alamos with a highlight presentation by Nobel Laureate K. A. Mueller (Switzerland). We also initiated a lively exchange program with the NSF Materials Science Center (UCSB) on the topic "Frontiers in Materials Science", and are members of the UC campus-wide program "Quantum Design and Synthesis of Novel Materials". The modeling tools we have assembled are proving directly relevant to our projects with Motorola on the subject of high-dielectric-constant ferroelectric materials.

Our research accomplishments have been substantial in the areas of metal-insulator-transitions, non-Fermi-liquid behavior, and local structure. Highlights of these accomplishments are given below. Details can be found in the publications listed at the end of this report.

We have made detailed studies of the interplays of electron-electron coupling, electron-lattice coupling and doping in strongly correlated organic and inorganic electronic materials.

In particular, in oxide perovskites, we have found that this interplay is responsible for strong tendencies toward intrinsic inhomogeneities of spin and charge distribution and of lattice distortion. This is responsible for novel states of matter with nanoscale phase separation properties and coexistence of competing broken-symmetries (charge-density-wave, spin-density-wave, spin-Peierls, charge-localized, etc.). The associated filamentary, percolative, dielectric breakdown, and related properties (such as poor metal and non-Fermi-liquid behavior) represent a quite different scenario than the large-scale homogeneous one assumed in much of conventional solid state and many-body physics: controlling the multiple fine-scales of length and associated dynamic scales, and using the specific functionalities they control will be a major science and technology thrust for the forseeable future.

Our research has demonstrated the fundamental role of electron-lattice coupling in "colossal magnetoresistant (CMR) manganite oxides," which undergo a novel metal-insulator transitions coupled with a magnetic-nonmagnetic transition [35, 36 37, 41, 42, 46, 48, 51]. We have achieved understanding of the role of the lattice on this transition, the effect of magnetic fields, localization effects of spin fluctuations, oxygen isotope effects, and aspects of glassy (i.e. multi-timescale) dynamics. Extensive comparisons with a variety of experimental data from Los Alamos researchers and elsewhere has been possible, including phonon and magnetic neutron scattering, extended x-ray fine structure, electron-spin-resonance, muon-spin-resonance, resonant ultrasound scattering and transport. Signatures of small- and intermediate-size polarons in the doped materials have been especially striking. The identification of the local variations of lattice structure around charges localized as polarons and mesoscopic polaron assemblies has been aided substantially by advances in x-ray and neutron scattering with high-intensity sources. These now permit the extraction of athermal local lattice distortions through pair-distribution-function (real space) and diffuse x-ray (wave-vector space) scattering. We have worked closely with experimental colleagues [37, 41] to develop new data analysis tools [49] to systematically and quantitatively extract this crucial local scale information, where essential electronic and magnetic functionalities emerge – and are almost totally lost in macroscopic or average measurements or modeling approaches.

Having developed the above framework and tools, it is recently becoming clear that closely related multiscale functionalities appear in many related complex electronic materials, and are set to change conventional philosophy in those materials. We have completed initial modeling and experimental data comparisons for nickelates [53], cuprate layered and ladder [56] compounds, organic charge-transfer chain compounds [57], and heavy-fermion compounds [58]. In all of these cases, there is growing evidence for non-

fermi-liquid behavior, quantum critical behavior, pseudogap behavior, and nanoscale spin-charge-lattice phase separation.

We have also completed totally new studies of nonlinear and nonadiabatic effects in prototypical models incorporating electron-lattice and electron-electron coupling [31, 40, 43, 53, 60, 61]. Particularly novel is our discovery of multi-phonon bound states (so-called "breather" states), and the stable combination of these states with excitons to form "breather-excitons" [53]. These fundamentally nonlinear and nonadiabatic phenomena have exciting prospects for localizing and transducing energy, and for enhancing nonlinear optical coefficients. They are now under very active exploration, experimentally and theoretically, in a number of organic, inorganic and even biological contexts – transition metal oxides, charge-transfer salts, organic-inorganic interfaces, myoglobin, etc.

We have developed new methods to calculate the properties of electron-phonon coupled systems (polarons), including dynamical quantum phonons. These methods have allowed us to calculate the ground state energy of a Holstein polaron to ten million times greater accuracy than any other published result. We have also calculated the energy and correlation functions at arbitrary momentum to high accuracy. We find an unusual phase transition in the first excited state between Raman active bound and unbound states of a polaron and an additional phonon[21]. Related methods were used to calculate the coherent quantum dynamics of a driven polaron far from equilibrium, and inelastic tunneling properties[9]. Results include a calculation of the oscillating phonon wake of a fast electron in a solid[13]. These calculations are a qualitative improvement on incoherent approximations based on rate equations. Results from these calculations are being applied to electrons tunneling through polymers, and to the dynamics of polaron formation as observed in fast time-resolved optical experiments. We have also calculated spin properties of CMR materials, obtained a simple strong-coupling picture of d-wave superconductivity[11], calculated magneto-thermoelectric transport properties of semimetals with applications to Ettingshausen refrigerators[15, 16, 17, 23], and properties of correlated electron (high-T_c and CMR) systems as observed by fast time-resolved optical experiments [14, 19].

We demonstrated striking experimental effects arising from competitions between broken-symmetries and the large-scale influences of even small and local perturbations. Our primary objective was to investigate the nature of superconducting states with broken time-reversal invariance [1, 2]. We focused our effort on the major issue of marginal stability of unconventional superconductors and on the role of impurities and external perturbations on the induction of the secondary components of the order parameter. We were able to show how the secondary components are generated near a magnetic impurity,

as in the case of nickel-doped bismuth 2212 superconductor [2]. We also investigated the role of stripe and phase separation on the structure of the superconducting order paramenter in correlated systems with competing interactions [65]. Additionally, we investigated the correlations between the superconducting transition temperature and the q-width of the peak at the antiferromagnetic wave vector, q (= π,π). We found a simple linear relation between the peak width and superconducting T_c (T_c=hv*q) with surprisingly small velocity (hv*=35meV.A) for the yttrium-barium-copper-oxygen superconductor.

We also showed the existence of the highly anisotropic impurity bound states in unconventional superconductors, such as d-wave superconductors [68, 69, 70, 73]. The energy position and real space shape of these impurity states offer a nontrivial probe of the pairing state in high temperature superconductors. The theory of these states, developed in collaboration with J.R. Schrieffer, D. J. Scalapino and M. Salkola, has become the motivation for extensive Scanning Tunneling Macroscopy studies of the impurity states at major centers such as University of Illinois (Urbana), IBM (Alamden), University of Hokkaido (Japan).

We also focused on the development and application of Chebyshev [29] and maximum entropy methods [24] for calculations with the extremely large (> 10^7 states) Hamiltonians relevant to many-body physics. Such methods provide linear scaling in the system size with controlled energy resolution, controlled statistical accuracy, and uniform convergence. They are most appropriate for calculating properties involving many eigenstates. They are complementary to Lanczos methods which are most appropriate for calculating specific extreme eigenstates. Quantities of interest include electronic energies [28], thermodynamics, spectral functions [25, 29], and Raman cross sections. Physics applications included spin systems [27], linear scaling electronic structure [26, 28], and quantum-breathers [52]. At this time, Chebyshev and maximum entropy methods have matured as a reliable and efficient way to systematically calculate physical properties of a wide variety of Hamiltonians.

Perhaps most significantly the ideas which motivated this project three years ago have now become the center of national science initiatives as well as major Los Alamos internal thrust discussions -- as witnessed by this year's National Academy Report "Science Serving Society", the recent new DOE Initiative "Complex and Collective Phenomena" and by complementary Los Alamos initiatives under the general rubric of "Complex Adaptive Matter". Of special note are the issues emerging as focuses in complex organic and inorganic electronic materials that are at the cutting edge for the future -- including intrinsic (multiscale) inhomogeneities in spin, charge and lattice properties and associated multi-

time-scale dynamics, and extreme sensitivities to small internal and external perturbations (doping, impurities, magnetic field, photoexcitation, etc.). These properties are the underpinning issues in the focuses on crossover phenomena and quantum critical behavior in many classes of organic and inorganic strongly correlated electronic materials, which are currently attracting such excitement at Los Alamos and internationally.

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MAJOR INVITED PRESENTATIONS

Trugman, S. A., Invited Talk on Polarons, at the Euroconference on Polarons: Condensation, Pairing, and Magnetism, Erice, Sicily, June 1998.

Trugman, S. A., Invited Talk on Colossal Magnetoresistance and Polarons, Michigan State University Conference on Manganites, July 1998.

Trugman, S. A., Invited Talks on Inelastic Quantum Transport and on Low Temperature Magnetic Properties of the Double Exchange Model, Aspen Center for Physics, July 1996.

Balatsky, A. V., "Impurities in d-wave Superconductors", Taiwan School on Correlated Electrons, Hsinchu, Taiwan, January 1998.

Balatsky, A. V., "Marginal Stability of d-wave Superconductors", Florida Japan-US Meeting), Tallahassee, Florida, March 1998; Stripes 98, Rome, Italy, June 1998; Polarons 98, Erice, Italy, June 1998; SCES98, Paris, France, July 1998.

Balatsky, A. V., "Spontaneous Parity and Time Reversal Violation in d-wave Superconductor", New Material and Mechanisms in Superconductivity, Baton Rouge, LA, February 1998 and Aspen Center for Physics, Aspen, CO, July 1998.

Bishop, A. R. International Conference on "Magnetoresistant Materials", Centro Atomico, Bariloche, Argentina, August 1998.

Bishop, A. R., Euroconference "Intrinsic Local Modes", Lyon, France, July 1998.

Bishop, A. R., Workshop on CMR Materials, Telluride, CO, July 1998.

Bishop, A. R., Euroconference "Polarons: condensation, pairing, magnetism", Erice, Sicily, June 1998.

Bishop, A. R., International Conference "Magnetoreistive manganite oxides", Melbourne, Australia, June 1998.

Bishop, A. R., International Conference "Progress and Challenges in Complexity", Okayama, Japan, April 1998.

Bishop, A. R., Euroconference "Lattice dynamics and phase transitions", Erice, Sicily, June 1997.

Bishop, A. R., International Workshop "Quantum phase transitions in spin systems and guage theories", Florence, Italy 1996.

Bishop, A. R., International Conference "Sin-Charge-Lattice effects in oxide perovskites", Tsukuba, Japan 1996.

Silver, R. N., U.S./India Joint Seminar on Bose-Einstein Condensation and Pairing Phenomena ``Bose Condensation Condensation in ^{4}He and Neutron Scattering", , Pune, India, December 1996

Silver, R. N., International Workshop on High Temperature Superconductivity: 10 Years After Its Discovery , ``Neutron Scattering Evidence for Bose Condensation in Superfluid ^{4}He", Jaipur, India, December 1996

Silver, R. N., Workshop on Maximum Entropy and Bayesian Methods, ``Chebyshev Moment Problems: Maximum Entropy and Kernel Polynomial Methods", Santa Fe, New Mexico, USA.

Silver, R. N., Coherent Approaches to Fluctuations ``Chebyshev Recursion Methods: Kernel Polynomials and Maximum Entropy"

Balatsky, A. V., Impurity Workshop, ``Absence of Quasiparticle Localization in Disordered d-wave Superconductor", University of Florida, February 1995.

Balatsky, A. V., ETH Zurich, ``Impurity Bound States in D-Wave Superconductors", January 1996.

Balatsky, A. V., APS March Meeting, "Impurity States and Impurity Bands in D-wave Superconductors", St. Louis, 1996.

Balatsky, A. V., Spectroscopies of Novel Superconductors, Cape Cod, ``Spontaneous Violation of Parity and Time Reversal in d-wave Superconductor with Magnetic Impurities", Sept 97,.

Balatsky, A. V., US-Japan meeting in Tallahassee, ``Spontaneous Violation of Parity and Time Reversal in d-wave Superconductor", March 98.